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Generalized local and nonlocal master equations for some stochastic processes☆

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ABSTRACT

In this paper, we present a study on generalized local and nonlocal equations for some stochastic processes. By considering the net flux change in a region determined by the transition probability, we derive the master equation to describe the evolution of the probability density function. Some examples, such as classical Fokker–Planck equations, models for Lévy process, and stochastic coagulation equations, are provided as illustrations. A particular application is a consistent derivation of coupled dynamical systems for spatially inhomogeneous stochastic coagulation processes.

1. Introduction

Given a stochastic process X_t, which may represent various processes such as the diffusion process, stochastic coagulation process, or continuous time random walk (CTRW), there are many methods to derive the evolution equation of its probability density function (PDF) $f = f(\mathbf{x}, t)$, which represents the probability that the system of interest is in the state $\mathbf{x}$ at time t. A general master equation in *differential* form may be written as [1]

$$f_t(\mathbf{x}, t') = \int_0^t \int_{\mathbb{R}^n} \Big[K(\mathbf{x}', \mathbf{x}, t-\tau) f(\mathbf{x}', \tau) - K(\mathbf{x}, \mathbf{x}', t-\tau) f(\mathbf{x}, \tau) \Big] \, d\mathbf{x}' d\tau, \tag{1.1}$$

where K is a *memory*-dependent nonlocal transition kernel [2] for general, and possibly non-Markovian, processes. For Markov processes which have no memory effect, Eq. (1.1) reduces to

$$f_t(\mathbf{x}, t) = \int_{\mathbb{R}^n} \Big[\gamma(\mathbf{x}', \mathbf{x}, t) f(\mathbf{x}', t) - \gamma(\mathbf{x}, \mathbf{x}', t) f(\mathbf{x}, t) \Big] \, d\mathbf{x}', \tag{1.2}$$

where $\gamma(\mathbf{x}', \mathbf{x}, t)$ denotes the transition rate from $\mathbf{x}'$ to $\mathbf{x}$ at time t. In the *discrete time* form, (1.2) is often reformulated as

$$f(\mathbf{x}, t) - f(\mathbf{x}, t') = \int_{\mathbb{R}^n} \Big[p(\mathbf{x}', t'; \mathbf{x}, t) f(\mathbf{x}', t') - p(\mathbf{x}, t'; \mathbf{x}', t) f(\mathbf{x}, t') \Big] \, d\mathbf{x}', \tag{1.3}$$

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where $p(\mathbf{x}', t'; \mathbf{x}, t)$ represents the transition probability (TP) of a particle moving from $\mathbf{x}'$ at time t' to $\mathbf{x}$ at time t; the first part of the right hand side represents the incoming flux and the second part is the outgoing flux. Notice that

$$\int p(\mathbf{x}, t'; \mathbf{x}', t) \mathrm{d}\mathbf{x}' = 1,$$

the master equation (1.3) can thus be equivalently interpreted as the Chapman–Kolmogorov equation (CKE). There have been many works on the study of the evolution of Markov processes using the CKE, see for instance [3,4]. In [5], a nonlinear Fokker–Planck equation (FPE) of Markov processes is derived from the master equation in the gain–loss form by characterizing the transition probability. Master equations can also be applied to study non-Markov processes. For example, an equivalence is established between generalized master equations and continuous time random walks in [1]. In general, for either Markov or non-Markov processes, the master equation is completely determined by the transition kernel. For example, Taylor expansion of transition probability on CKE can be applied to derive the evolution equation of some Markov processes, but such a technique does not apply when there is nonlocal or non-Markovian effect [3,4]. On the other hand, it is possible to derive the evolution equation from the master equation (1.3) through a Taylor expansion on the PDF instead of the transition kernel. In this paper, we will mainly focus on the Markov process though our method can be extended to non-Markov process by taking into account the time integral over memory kernel terms. We present the derivations of the evolution equations for some Markov stochastic processes from the master equation in gain–loss form (1.3). Our approach is to consider a nonlocal flux as that in [6–8]. A key ingredient is to obtain an expression of the transition probability (TP) either explicitly or implicitly that is valid for both the local and nonlocal settings associated with complex transport and diffusion processes. We verify the derivations in the later sections. A particular application is a consistent derivation of spatial inhomogeneous stochastic coagulation process. In what follows, we present the generalized master equation framework in Section 1.1; then we apply it to some classical stochastic processes in Section 2 and relating stochastic processes involving nonlocal effect with nonlocal master equations in Section 3; this generalized master equation framework can be unified under the recently developed nonlocal vector calculus, and the details are given in Section 4; furthermore in Section 5, we establish rigorously a result on joint stochastic processes and show how the generalized master equation can be applicable to certain type of coupled dynamical system.

1.1. Generalized master equation framework

To present our approach, let us review the concept of conservation law. Assume $f(\mathbf{x}, t)$ is the PDF of a physical quantity $X = X_t$ such as heat, energy and mass. The total amount of X in a region $\Omega \in \mathbb{R}^n$ at time t is

$$\int_{\mathbf{x}\in\Omega} f(\mathbf{x}, t)\, \mathrm{d}\mathbf{x}.$$

X is conserved if it is only gained or lost through the domain boundaries without external sources. Let the vector field $\mathbf{F}(\mathbf{x}, t)$ be the flux. The conservation law implies that the rate of change of the density plus the divergence of the flux is equal to 0,

$$\frac{\partial f}{\partial t} + \nabla_x \cdot \mathbf{F} = 0. \tag{1.4}$$

The transport equation, the diffusion equation and the wave equation, can be derived from the principle of conservation law given the explicit form of the flux. Nevertheless, as discussed in [7,8], the flux $\mathbf{F}$ adopted in (1.4) is a local notion which is not always suitable for a general process X_t. On the other hand, it is possible to determine the TP $p(\mathbf{x}', t'; \mathbf{x}, t)$ which represents the probability that a particle is transferred from $\mathbf{x}'$ at time t' to $\mathbf{x}$ at time t. In [8], a notion of nonlocal flux was introduced to account for more general, nonlocal spatial interactions. The discussion here is intended for time-dependent processes but the principle is similar. We begin by rewriting the conservation law in a gain–loss form. Given a stochastic process X_t with its PDF $f(\mathbf{x}, t)$ representing a conserved physical quantity which is only gained or lost through the domain boundaries, then the quantity change in this domain Ω from time t' to t ($t' < t$) equals the net flux. The generalized equation of conservation law is written as

$$\int_{\mathbf{x}\in\Omega} f(\mathbf{x}, t)\, \mathrm{d}\mathbf{x} - \int_{\mathbf{x}\in\Omega} f(\mathbf{x}, t')\, \mathrm{d}\mathbf{x} = \mathcal{F}(\Omega, t', t) = \mathcal{F}^+(\Omega, t', t) - \mathcal{F}^-(\Omega, t', t), \tag{1.5}$$

where $\mathcal{F}^+$ and $\mathcal{F}^-$ represent the incoming flux and outgoing flux in the region Ω from t' to t respectively, and $\mathcal{F}(\Omega, t', t)$ is the net (*nonlocal*) flux for the region Ω or between Ω and Ω^c (the complement of Ω). More specifically, we write the incoming flux $\mathcal{F}^+(\Omega, t', t)$ in the region Ω in terms of the TP

$$\mathcal{F}^+(\Omega, t', t) = \int_{\mathbf{x}\in\Omega} \int_{\mathbf{x}'\in\Omega^c} p(\mathbf{x}', t'; \mathbf{x}, t) f(\mathbf{x}', t')\, \mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}, \tag{1.6}$$

and the outgoing flux $\mathcal{F}^-(\Omega, t', t)$ by

$$\mathcal{F}^-(\Omega, t', t) = \int_{\mathbf{x}\in\Omega} \int_{\mathbf{x}'\in\Omega^c} p(\mathbf{x}, t'; \mathbf{x}', t) f(\mathbf{x}, t')\, \mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{x}. \tag{1.7}$$